9

X-RAY STUDY OF *p*-ANISIDINE

M. Y. KHAN AND Y. MISRA

DEPARTMENT OF PHYSICS, UNIVERSITY OF GORAKHPUR,

GORAKHPUR (INDIA)

(*Received April* 1, 1966)

The substance *p*-Anisidine (alternative name *p*-amino anisol) C_7H_9NO, finds an important place in the synthesis of various colorants (Chernuikh, 1935) and drugs (Smith and Burnett, 1949). Good single crystals, of the substance were obtained from its saturated solution in ethanol under controlled evaporation and repeated crystallisation. The crystals are long prismatic in shape with brownish tinge, and show four faces parallel to the needle direction. Goniometric observations from the crystal suggest that it belongs to the monoclinic system. The faces (001) and (100) are very well developed and prominent in all the crystals. The interfacial angles $(100)\wedge(001)$ and $(001)\wedge(\bar{1}00)$ are 74°18′ and 105°42′, are in good agreement with the calculated values of 74°17′ and 105°43′ respectively.

The axial parameters of the unit cell from the oscillation photographs were refined by the method of least squares using high angle spots on the zero layer Weissenberg photographs (Hugos, Yakel, and Freeman, 1961). The camera diameter was standardised with the help of aluminium wire powder pattern superimposed on the oscillation and the zero layer Weissenberg photographs. Unfiltered copper radiation from Machelett tube at 25KV, 10mA was used The monoclinic angle β was determined from the zero layer Weissenberg photograph along the unique axis and was further refined by the method of angular lag from first and second layer equi-inclination Weissenberg photographs (Buerger, 1942).

The density of crystals was measured by floation method The observed density is $D_m = 1.20\,g.\,cm^{-3}$ against the reported density $D = 1.08 g.\,cm^{-3}$. (Hilbron, and Bunbury, 1934). The number of molecules per unit cell is 4 and the calculated density is $D_x = 1.21 g\ cm^{-3}$ which is in good agreement with the observed value. Equi-inclination Weissenberg photographs were taken along the three crystallographic directions and the spots were indexed with the help of lattice row templates (Schneider, 1928) and checked by direct calculations for the Bragg angles.

From the study of indexed reflections, it is found that all (*hkl*) reflections are present. The systematic extinctions are (*hol*) with *l* odd and (*oko*) with *k* odd.

It shows that the lattice is primitive, the unique axis is a screw axis and the symmetry plane is a glide plane with glide component along c. These conditions enable us to assign the space group $C^5_{2h}-P2_1/c$.

The crystal data as determined from this X-ray study are given below :

$a = 7.78 \pm 0.01$ Å.	$D_m = 1.20 \text{g.cm}^{-3}$
$b = 5.60 \pm 0.01$ Å	$D_x = 1.21 \text{g. cm}^{-3}$
$c = 16.08 \pm 0.02$ Å.	$Z = 4$
$\beta = 105°22'$.	$F(000) = 264$.
$Vc = 674.44$ Å^3.	
$\mu = 6.69$ cm.	

for CuK_α radiation ($\lambda = 1.5418$ Å).

Further work on complete structure determination of *p*-anisidine is in progress and will be published shortly

The authors are indebted to Prof. D Sharma for his keen interest and Dr. P Srivastava for his guidance and supervision of the work. Financial assistance from the Council of Scientific and Industrial Research, New Delhi, is also gratefully acknowledged.

REFERENCES

Buerger, M J , 1942, '*X-ray Crystallography*. (Wiley, N Y) pp 380.
Cheramukh, E V , 1935 *Russ* , **41**, 615
Hodbron, I , Bunbury, H. M., 1934, '*Dictionary of Organic Compounds*', (London)
Hughes, E W , Yakel, H L , and Freeman, H C , 1961, *Acta Cryst* **14**, 345.
Schneider, W., 1928, *Zeit. fur Kristallogr.* (*A*), **69**, 41.
Smith, N. C., and Burnett, D., 1949, *Jr J. Econ Entomol.* **42**, 439.